Quantum Mechanics in Pℏase Space

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Abstract

Ever since Werner Heisenberg's 1927 paper on uncertainty, there has been considerable hesitancy in simultaneously considering positions and momenta in quantum contexts, since these are incompatible observables. But this persistent discomfort with addressing positions and momenta jointly in the quantum world is not really warranted, as was first fully appreciated by Hilbrand Groenewold and José Moyal in the 1940s. While the formalism for quantum mechanics in phase space was wholly cast at that time, it was not completely understood nor widely known — much less generally accepted — until the late 20th century.

When Feynman first unlocked the secrets of the path integral formalism and presented them to the world, he was publicly rebuked [8]: "It was obvious, Bohr said, that such trajectories violated the uncertainty principle."

However, in this case,[1] Bohr was wrong. Today path integrals are universally recognized and widely used as an alternative framework to describe quantum behavior, equivalent to although conceptually distinct from the usual Hilbert space framework, and therefore completely in accord with Heisenberg's uncertainty principle. The different points of view offered by the Hilbert space and path integral frameworks combine to provide greater insight and depth of understanding.

Similarly, many physicists hold the conviction that classical-valued position and momentum variables should not be simultaneously employed in any meaningful formula expressing quantum behavior, simply because this would also seem to violate the uncertainty principle (see Dirac).

However, they too are wrong. Quantum mechanics (QM) *can* be consistently and autonomously formulated in phase space, with c-number position and momentum variables simultaneously placed on an equal footing, in a way that fully respects Heisenberg's principle. This other quantum framework is equivalent to both the Hilbert space approach and the path integral formulation. Quantum mechanics in phase space (QMPS) thereby gives a third point of view which provides still more insight and understanding.

What follows is the somewhat erratic story of this third formulation.

R Feynman

N Bohr

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[1]Unlike the more famous cases where Bohr criticised thought experiments proposed by Einstein, at the 1927 and 1930 Solvay Conferences.

The foundations of this remarkable picture of quantum mechanics were laid out by H Weyl and E Wigner around 1930. But the full, self-standing theory was put together in a crowning achievement by two unknowns, at the very beginning of their physics careers, independently of each other, during World War II: H Groenewold in Holland and J Moyal in England (see Groenewold and Moyal). It was only published after the end of the war, under not inconsiderable adversity, in the face of opposition by established physicists; and it took quite some time for this uncommon achievement to be appreciated and utilized by the community.[2]

H Weyl

The net result is that quantum mechanics works smoothly and consistently in phase space, where position coordinates and momenta blend together closely and symmetrically. Thus, sharing a common arena and language with classical mechanics [14], QMPS connects to its classical limit more naturally and intuitively than in the other two familiar alternate pictures, namely, the standard formulation through operators in Hilbert space, or the path integral formulation.

Still, as every physics undergraduate learns early on, classical phase space is built out of "c-number" position coordinates and momenta, x and p, ordinary commuting variables characterizing physical particles; whereas such observables are usually represented in quantum theory by operators that do not commute. How then can the two be reconciled? The ingenious technical solution to this problem was provided by Groenewold in 1946, and consists of a special binary operation, the $\star$-product (see Star Product), which enables x and p to maintain their conventional classical interpretation, but which also permits x and p to combine more subtly than conventional classical variables; in fact to combine in a way that is *equivalent* to the familiar operator algebra of Hilbert space quantum theory.

W Heisenberg and E Wigner

Nonetheless, expectation values of quantities measured in the lab (observables) are computed in this picture of quantum mechanics by simply taking integrals of conventional functions of x and p with a quasi-probability density in phase space, the Wigner function — essentially the density matrix in this picture. But, unlike a Liouville probability density of classical statistical mechanics, this density can take provocative negative values and, indeed, these can be reconstructed from lab measurements [11].

How does one interpret these "negative probabilities" in phase space? The answer is that, like a magical invisible mantle, the uncertainty principle manifests itself in this picture in unexpected but quite powerful ways, and prevents the formulation of unphysical questions, let alone paradoxical answers (see Uncertainty Principle).

Remarkably, the phase-space formulation was reached from rather different, indeed, apparently unrelated, directions. To the extent this story has a beginning, this may well have been H Weyl's remarkably rich 1927 paper [18] (reprinted in [20]) shortly after the triumphant formulation of conventional QM. This paper introduced the correspondence of phase-space functions to "Weyl-ordered" operators in Hilbert space. It relied on a systematic, completely symmetrized ordering scheme of noncommuting operators $\boldsymbol{X}$ and $\boldsymbol{P}$.

Eventually it would become apparent that this was a mere change of representation. But as expressed in his paper at the time [18], Weyl believed that this map, which now bears his name, is "the" quantization prescription — superior to other prescriptions — the elusive bridge extending classical mechanics to the operators of the broader quantum theory containing it; effectively, then, some extraordinary "right way" to a "correct" quantum theory.

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[2]Perhaps this is because it emerged nearly simultaneously with the path integral and associated diagrammatic methods of Feynman, whose flamboyant application of those methods to the field theory problems of the day captured the attention of physicists worldwide, and thus overshadowed other theoretical developments.

However, Weyl's correspondence *fails* to transform the square of the classical angular momentum to its accepted quantum analog; and therefore it was soon recognized to be an elegant, but not intrinsically special quantization prescription. As physicists slowly became familiar with the existence of different quantum systems sharing a common classical limit, the quest for the right way to quantization was partially mooted.

In 1931, in establishing the essential uniqueness of Schrödinger's representation in Hilbert space, von Neumann utilized the Weyl correspondence as an equivalent abstract representation of the Heisenberg group in the Hilbert space operator formulation. For completeness' sake, ever the curious mathematician's foible, he worked out the analog (isomorph) of operator multiplication in phase space. He thus effectively discovered the convolution rule governing the noncommutative composition of the corresponding phase-space functions — an early version of the ⋆-product.

Nevertheless, possibly because he did not use it for anything at the time, von Neumann oddly ignored his own early result on the ⋆-product and just proceeded to postulate correspondence rules between classical and quantum mechanics in his very influential 1932 book on the foundations of QM [13]. In fact, his ardent follower, Groenewold, would use the ⋆-product to show some of the expectations formed by these rules to be untenable, 15 years later. But we are getting ahead of the story.

J von Neumann

Very soon after von Neumann's paper appeared, in 1932, Eugene Wigner approached the problem from a completely different point of view, in an effort to calculate quantum corrections to classical thermodynamic (Boltzmann) averages. Without connecting it to the Weyl correspondence, Wigner introduced his eponymous function (see Wigner Functions), a distribution which controls quantum-mechanical diffusive flow in phase space, and thus specifies quantum corrections to the Liouville density of classical statistical mechanics.

As Groenewold and Moyal would find out much later, it turns out that this WF maps to the density matrix (up to multiplicative factors of $\hbar$) under the Weyl map. Thus, without expressing awareness of it, Wigner had introduced an explicit illustration of the inverse map to the Weyl map, now known as the Wigner map.

Wigner also noticed the WF would assume negative values, which complicated its conventional interpretation as a probability density function. However — perhaps unlike his sister's husband — in time Wigner grew to appreciate that the negative values of his function were an asset, and not a liability, in ensuring the orthogonality properties of the formulation's building blocks, the "stargenfunctions" (see Simple Harmonic Oscillator).

Wigner further worked out the dynamical evolution law of the WF, which exhibited the nonlocal convolution features of ⋆-product operations, and violations of Liouville's theorem. But, perhaps motivated by practical considerations, he did not pursue the formal and physical implications of such operations, at least not at the time. Those and other decisive steps in the formulation were taken by two young novices, independently, during World War II.

In 1946, based on his wartime PhD thesis work, much of it carried out in hiding, Hip Groenewold published a decisive paper, in which he explored the consistency of the classical-quantum correspondences envisioned by von Neumann. His tool was a fully mastered formulation of the Weyl correspondence as an invertible transform, rather than as a consistent quantization rule. The crux of this isomorphism is the celebrated ⋆-product in its modern form.

Use of this product helped Groenewold demonstrate how Poisson brackets contrast crucially to quantum commutators ("Groenewold's Theorem"). In effect, the Wigner map of quantum commutators is a generalization of Poisson brackets, today called Moyal brackets (perhaps unfairly, given that Groe-

newold's work appeared first), which contains Poisson brackets as their classical limit (technically, a Wigner-Inonü Lie-algebra contraction). By way of illustration, Groenewold further worked out the harmonic oscillator WFs. Remarkably, the basic polynomials involved turned out to be those of Laguerre, and not the Hermite polynomials utilized in the standard Schrödinger formulation! Groenewold had crossed over to a different continent.

At the very same time, in England, Joe Moyal was developing effectively the same theory from a yet different point of view, landing at virtually the opposite coast of the same continent. He argued with Dirac on its validity (see Dirac) and only succeeded in publishing it, much delayed, in 1949. With his strong statistics background, Moyal focussed on all expectation values of quantum operator monomials, $\boldsymbol{X}^n \boldsymbol{P}^m$, symmetrized by Weyl ordering, expectations which are themselves the numerically valued (c-number) building blocks of every quantum observable measurement.

Moyal saw that these expectation values could be generated out of a *classical-valued characteristic function in phase space*, which he only much later identified with the Fourier transform used previously by Wigner. He then appreciated that many familiar operations of standard quantum mechanics could be apparently bypassed. He reassured himself the uncertainty principle was incorporated in the structure of this characteristic function, and that it indeed constrained expectation values of "incompatible observables." He interpreted subtleties in the diffusion of the probability fluid and the "negative probability" aspects of it, appreciating that negative probability is a microscopic phenomenon.

Today, students of QMPS routinely demonstrate as an exercise that, in $2n$-dimensional phase space, domains where the WF is solidly negative cannot be significantly larger than the minimum uncertainty volume, $(\hbar/2)^n$, and are thus not amenable to direct observation — only indirect inference [11].

Less systematically than Groenewold, Moyal also recast the quantum time evolution of the WF through a deformation of the Poisson bracket into the Moyal bracket, and thus opened up the way for a direct study of the semiclassical limit $\hbar \to 0$ as an asymptotic expansion in powers of $\hbar$ — "direct" in contrast to the methods of taking the limit of large occupation numbers, or of computing expectations of coherent states (see Classical Limit). The subsequent applications paper of Moyal with the eminent statistician Maurice Bartlett also appeared in 1949, almost simulaneously with Moyal's fundamental general paper. There, Moyal and Bartlett calculate propagators and transition probabilities for oscillators perturbed by time-dependent potentials, to demonstrate the power of the phase-space picture.

M Bartlett

By 1949 the formulation was complete, although few took note of Moyal's and especially Groenewold's work. And in fact, at the end of the war in 1945, a number of researchers in Paris, such as J Yvon and J Bass, were also rediscovering the Weyl correspondence and converging towards the same picture, albeit in smaller, hesitant, discursive, and considerably less explicit steps (see [20] for a guide to this and related literature).

Important additional steps were subsequently carried out by T Takabayasi (1954), G Baker (1958, his thesis), D Fairlie (1964), and R Kubo (1964) (again, see [20]). These researchers provided imaginative applications and filled-in the logical autonomy of the picture — the option, in principle, to derive the Hilbert-space picture from it, and not vice versa. The completeness and orthogonality structure of the eigenfunctions in standard QM is paralleled in a delightful shadow-dance, by QMPS $\star$-operations (see Pure States and Star Products, and Simple Harmonic Oscillator).

D Fairlie

QMPS can obviously shed light on subtle quantization problems as the comparison with classical theories is more systematic and natural. Since the variables involved are the same in both classical and quantum cases, the connection
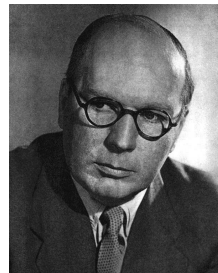
to the classical limit as $\hbar \to 0$ is more readily apparent (see Classical Limit). But beyond this and self-evident pedagogical intuition, what is this alternate formulation of QM and its panoply of satisfying mathematical structures good for?

It is the natural language to describe quantum transport, and to monitor decoherence of macroscopic quantum states, in interaction with the environment, a pressing central concern of quantum computing [15]. It can also serve to analyze and quantize physics phenomena unfolding in an hypothesized *noncommutative spacetime* with various noncommutative geometries [17]. Such phenomena are most naturally described in Groenewold's and Moyal's language.

However, it may be fair to say that, as was true for the path integral formulation during the first few decades of its existence, the best QMPS "killer apps" are yet to come.

Work by CoBrA artist Mogens Balle (1921-1988).

Acknowledgement

Appendices

The following supplements expand on the discussion in the text. The first three are historical commentaries, including biographical material, while the remaining supplements deal with elementary technical aspects of QMPS.

Dirac

A representative, indeed *authoritative*, opinion, dismissing even the suggestion that quantum mechanics can be expressed in terms of classical-valued phase space variables, was expressed by Paul Dirac in a letter to Joe Moyal on 20 April 1945 (see p 135, [1]). Dirac said, "I think it is obvious that there cannot be any distribution function $F(p, q)$ which would give correctly the mean value of any $f(p, q)$ ..." He then tried to carefully explain why he thought as he did, by discussing the underpinnings of the uncertainty relation.

However, in this instance, Dirac's opinion was wrong, and unfounded, despite the fact that he must have been thinking about the subject since publishing some preliminary work along these lines many years before [3]. In retrospect,

it is Dirac's unusual misreading of the situation that is obvious, rather than the non-existence of $F(p, q)$.

Perhaps the real irony here is that Dirac's brother-in-law, Eugene Wigner, had already constructed such an $F(p, q)$ several years earlier [19]. Moyal eventually learned of Wigner's work and brought it to Dirac's attention in a letter dated 21 August 1945 (see p 159, [1]).

Nevertheless, the historical record strongly suggests that Dirac held fast to his opinion that quantum mechanics could *not* be formulated in terms of classical-valued phase space variables. For example, Dirac made no changes when discussing the von Neumann density operator, $\boldsymbol{\rho}$, on p 132 in the final edition of his book [5]. Dirac maintained "Its existence is rather surprising in view of the fact that phase space has no meaning in quantum mechanics, there being no possibility of assigning numerical values simultaneously to the q's and p's." This statement completely overlooks the fact that the Wigner function $F(p, q)$ is precisely a realization of $\boldsymbol{\rho}$ in terms of numerical-valued q's and p's.

But how could it be, with his unrivaled ability to create elegant theoretical physics, Dirac did *not* seize the opportunity so unmistakably laid before him, by Moyal, to return to his very first contributions to the theory of quantum mechanics and examine in greater depth the relation between classical Poisson brackets and quantum commutators? We will probably never know beyond any doubt — yet another sort of uncertainty principle — but we are led to wonder if it had to do with some key features of Moyal's theory at that time. First, in sharp contrast to Dirac's own operator methods, in its initial stages QMPS theory was definitely *not* a pretty formalism! And, as is well known, beauty was one of Dirac's guiding principles in theoretical physics.

Moreover, the logic of the early formalism was not easy to penetrate. It is clear from his correspondence with Moyal that Dirac did not succeed in cutting away the formal undergrowth to clear a precise conceptual path through the theory behind QMPS, or at least not one that *he* was eager to travel again.[3]

One of the main reasons the early formalism was not pleasing to the eye, and nearly impenetrable, may have had to do with another key aspect of Moyal's 1945 theory: Two constructs may have been missing. Again, while we cannot be absolutely certain, we *suspect* the star product and the related bracket were both absent from Moyal's theory *at that time.* So far as we can tell, neither of these constructs appears in any of the correspondence between Moyal and Dirac. In fact, the product itself is not even contained in the published form of Moyal's work that appeared four years later [12], although the antisymmetrized version of the product — the so-called Moyal bracket — is articulated in that work as a generalization of the Poisson bracket,[4] after first being used by Moyal to express the time evolution of $F(p, q; t)$.[5] Even so, we are not aware of any historical evidence that Moyal *specifically* brought his bracket to Dirac's attention.

Thus, we can hardly avoid speculating, had Moyal communicated *only the contents of his single paragraph about the generalized bracket*[6] to Dirac, the latter would have recognized its importance, as well as its beauty, and the discussion between the two men would have acquired an altogether different tone. For, as Dirac wrote to Moyal on 31 October 1945 (see p 160, [1]), "I think your kind of work would be valuable only if you can put it in a very neat form." The Groenewold product and the Moyal bracket do just that.[6]

P Dirac

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[3]Although Dirac did pursue closely related ideas, at least once [4], in his contribution to Bohr's festschrift.

[4]See Eqn (7.10) and the associated comments in the last paragraph of §7, p 106, [12].

[5]See Eqn (7.8), [12]. Granted, the equivalent of that equation was already available in [19], but Wigner did *not* make the sweeping generalization offered by Moyal's Eqn (7.10).

[6]In any case, by then Groenewold had already found the star product, as well as the related bracket, by taking Weyl's and von Neumann's ideas to their logical conclusion, and had it all published [9] in the time between Moyal's and Dirac's last correspondence and the appearance of [12, 2], wherein discussions with Groenewold are acknowledged by Moyal.

Hilbrand Johannes Groenewold

29 June 1910 - 23 November 1996[7]

Hip Groenewold was born in Muntendam, The Netherlands. He studied at the University of Groningen, from which he graduated in physics with subsidiaries in mathematics and mechanics in 1934.

In that same year, he went of his own accord to Cambridge, drawn by the presence there of the mathematician John von Neumann, who had given a solid mathematical foundation to quantum mechanics with his book *Mathematische Grundlagen der Quantenmechanik*. This period had a decisive influence on Groenewold's scientific thinking. During his entire life, he remained especially interested in the interpretation of quantum mechanics (e.g. some of his ideas are recounted in [16]). It is therefore not surprising that his PhD thesis, which he completed eleven years later, was devoted to this subject [9]. In addition to his revelation of the star product, and associated technical details, Groenewold's achievement in his thesis was to escape the cognitive straight-jacket of the mainstream view that the defining difference between classical mechanics and quantum mechanics was the use of c-number functions and operators, respectively. He understood that these were only habits of use and in no way restricted the physics.

Ever since his return from England in 1935 until his permanent appointment at theoretical physics in Groningen in 1951, Groenewold experienced difficulties finding a paid job in physics. He was an assistant to Zernike in Groningen for a few years, then he went to the Kamerlingh Onnes Laboratory in Leiden, and taught at a grammar school in the Hague from 1940 to 1942. There, he met the woman whom he married in 1942. He spent the remaining war years at several locations in the north of the Netherlands. In July 1945, he began work for another two years as an assistant to Zernike. Finally, he worked for four years at the KNMI (Royal Dutch Meteorological Institute) in De Bilt.

During all these years, Groenewold never lost sight of his research. At his suggestion upon completing his PhD thesis, in 1946, Rosenfeld, of the University of Utrecht, became his promoter, rather than Zernike. In 1951, he was offered a position at Groningen in theoretical physics: First as a lecturer, then as a senior lecturer, and finally as a professor in 1955. With his arrival at the University of Groningen, quantum mechanics was introduced into the curriculum.

In 1971 he decided to resign as a professor in theoretical physics in order to accept a position in the Central Interfaculty for teaching Science and Society. However, he remained affiliated with the theoretical institute as an extraordinary professor. In 1975 he retired.

In his younger years, Hip was a passionate puppet player, having brought happiness to many children's hearts with beautiful puppets he made himself. Later, he was especially interested in painting. He personally knew several painters, and owned many of their works. He was a great lover of the after-war CoBrA art. This love gave him much comfort during his last years.
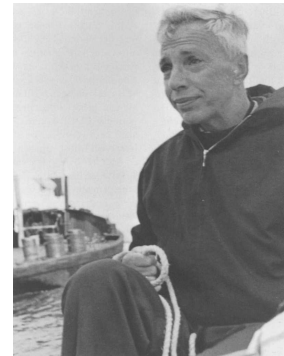
H Groenewold

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[7]The material presented here contains statements taken from a previously published obituary [10].

José Enrique Moyal

1 October 1910 - 22 May 1998[8]

Joe Moyal was born in Jerusalem and spent much of his youth in Palestine. He studied electrical engineering in France, at Grenoble and Paris, in the early 1930s. He then worked as an engineer, later continuing his studies in mathematics at Cambridge, statistics at the Institut de Statistique, Paris, and theoretical physics at the Institut Henri Poincaré, Paris.

After a period of research on turbulence and diffusion of gases at the French Ministry of Aviation in Paris, he escaped to London at the time of the German invasion in 1940. The eminent writer C.P. Snow, then adviser to the British Civil Service, arranged for him to be allocated to de Havilland's at Hatfield, where he was involved in aircraft research into vibration and electronic instrumentation.

During the war, hoping for a career in theoretical physics, Moyal developed his ideas on the statistical nature of quantum mechanics, initially trying to get Dirac interested in them, in December 1940, but without success. After substantial progress on his own, his poignant and intense scholarly correspondence with Dirac (Feb 1944 to Jan 1946, reproduced in [1]) indicates he was not aware, at first, that his phase-space statistics-based formulation was actually equivalent to standard QM. Nevertheless, he soon appreciated its alternate beauty and power. In their spirited correspondence, Dirac patiently but insistently recorded his reservations, with mathematically trenchant arguments, although lacking essential appreciation of Moyal's novel point of view: A radical departure from the conventional Hilbert space picture [12]. The correspondence ended in anticipation of a Moyal colloquium at Cambridge in early 1946.

That same year, Moyal's first academic appointment was in Mathematical Physics at Queen's University Belfast. He was later a lecturer and senior lecturer with M.S. Bartlett in the Statistical Laboratory at the University of Manchester, where he honed and applied his version of quantum mechanics [2].

In 1958, he became a Reader in the Department of Statistics, Institute of Advanced Studies, Australian National University, for a period of 6 years. There he trained several graduate students, now eminent professors in Australia and the USA. In 1964, he returned to his earlier interest in mathematical physics at the Argonne National Laboratory near Chicago, coming back to Macquarie University as Professor of Mathematics before retiring in 1978.

Joe's interests were broad: He was an engineer who contributed to the understanding of rubber-like materials; a statistician responsible for the early development of the mathematical theory of stochastic processes; a theoretical physicist who discovered the "Moyal bracket" in quantum mechanics; and a mathematician who researched the foundations of quantum field theory. He was one of a rare breed of mathematical scientists working in several fields, to each of which he made fundamental contributions.

J Moyal

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[8]The material presented here contains statements taken from a previously published obituary [7].

The *star product* is the Weyl correspondent of the Hilbert space operator product, and was developed through the work of many over a number of years: H Weyl (1927), J von Neumann (1931), E Wigner (1932), H Groenewold (1946), J Moyal (1949), and G Baker (1958), as well as more recent work to construct the product on general manifolds (reprinted in [20], along with related papers). There are useful integral and differential realizations of the product:

$$f \star g = \int \frac{dx_1 dp_1}{2\pi\,(\hbar/2)} \int \frac{dx_2 dp_2}{2\pi\,(\hbar/2)}\; f\,(x+x_1, p+p_1)\;g\,(x+x_2, p+p_2)\;\exp\left(\frac{i}{\hbar/2}\,(x_1 p_2 - x_2 p_1)\right)\;,$$

$$x_1 p_2 - x_2 p_1 = \text{Area}\,(1,2\ \text{parallelogram})\;,\quad \hbar/2 = \text{Planck Area} = \min\,(\Delta x \Delta p)\;,$$

$$f \star g = f\,(x,p)\;\exp\left(\overleftarrow{\partial_x}\,\frac{i\hbar}{2}\,\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\,\frac{i\hbar}{2}\,\overrightarrow{\partial_x}\right)\;g\,(x,p)\;,$$

$$
\begin{aligned}
f \star g &= f\left(x + \frac{1}{2}i\hbar\,\overrightarrow{\partial_p}\,,\; p - \frac{1}{2}i\hbar\,\overrightarrow{\partial_x}\right)\;g\,(x,p)\\
&= f\,(x,p)\;g\left(x - \frac{1}{2}i\hbar\,\overleftarrow{\partial_p}\,,\; p + \frac{1}{2}i\hbar\,\overleftarrow{\partial_x}\right)\\
&= f\left(x + \frac{1}{2}i\hbar\,\overrightarrow{\partial_p}\,,\; p\right)\;g\left(x - \frac{1}{2}i\hbar\,\overleftarrow{\partial_p}\,,\; p\right)\\
&= f\left(x, p - \frac{1}{2}i\hbar\,\overrightarrow{\partial_x}\right)\;g\left(x, p + \frac{1}{2}i\hbar\,\overleftarrow{\partial_x}\right)\;.
\end{aligned}
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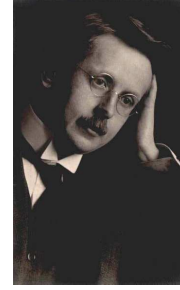
H Weyl

The *Moyal bracket*, $\{\{f,g\}\} = \frac{1}{i\hbar}\,[f,g]_\star$, is essentially just the antisymmetric part of a star product, where

$$[f,g]_\star \overset{\text{defn.}}{=} f \star g - g \star f\;.$$

This provides a homomorphism with commutators of operators, e.g. $[x,p]_\star = i\hbar$.

Wigner's original definition of his eponymous function was (Eqn(5) in [19])

$$\mathcal{P}\left(x_1, \cdots, x_n; p_1, \cdots, p_n\right) = \left(\frac{1}{\hbar\pi}\right)^n \int_{-\infty}^{\infty} \cdots \int dy_1 \cdots dy_n \psi\left(x_1 + y_1 \cdots x_n + y_n\right)^*$$
$$\psi\left(x_1 - y_1 \cdots x_n - y_n\right) e^{2i(p_1 y_1 + \cdots + p_n y_n)/\hbar} \ .$$

So defined, Wigner functions (WFs) *reside in phase space*.

WFs are the Weyl-correspondents of von Neumann's density operators, ρ. Thus, in terms of Hilbert space position and momentum *operators* $\boldsymbol{X}$ and $\boldsymbol{P}$, we have[9]

$$\rho = \frac{\hbar^n}{(2\pi)^{2n}} \int d^n\tau \, d^n\sigma \, d^n x \, d^n p \, \mathcal{P}\left(x_1, \cdots, x_n; p_1, \cdots, p_n\right) \exp\left(i\tau \cdot (\boldsymbol{P} - p) + i\sigma \cdot (\boldsymbol{X} - x)\right) \ .$$

In one x and one p dimension, denoting the WF by $F(x, p)$ instead of $\mathcal{P}$ (in deference to the momentum operator $\boldsymbol{P}$), we have

$$F(x, p) = \frac{1}{\pi\hbar} \int dy \, \langle x + y| \, \rho \, |x - y\rangle \, e^{-2ipy/\hbar} \ ,$$
$$\langle x + y| \, \rho \, |x - y\rangle = \int dp \, F(x, p) \, e^{2ipy/\hbar} \ ,$$
$$\rho = 2 \int dx dy \int dp \, |x + y\rangle \, F(x, p) \, e^{2ipy/\hbar} \, \langle x - y| \ .$$

For a quantum mechanical "pure state"

$$F(x, p) = \frac{1}{\pi\hbar} \int dy \, \psi(x + y) \, \psi^*(x - y) \, e^{-2ipy/\hbar} \ ,$$
$$\psi(x + y) \, \psi^*(x - y) = \int dp \, F(x, p) \, e^{2ipy/\hbar} \ ,$$
$$\rho = |\psi\rangle \langle\psi| \ ,$$

where as usual, $\psi(x + y) = \langle x + y \, |\psi\rangle$, $\langle\psi| \, x - y\rangle = \psi^*(x - y)$. Direct application of the Cauchy–Bunyakovsky–Schwarz inequality to the first of these pure-state relations gives

$$|F(x, p)| \le \frac{1}{\pi\hbar} \int dy \, |\psi(y)|^2 \ .$$

So, for normalized states with $\int dy \, |\psi(y)|^2 = 1$, we have the bounds

$$-\frac{1}{\pi\hbar} \le F(x, p) \le \frac{1}{\pi\hbar} \ .$$

Such normalized states therefore cannot give probability spikes (e.g. Dirac deltas) without taking the classical limit $\hbar \to 0$. The corresponding bound in $2n$ phase-space dimensions is given by the same argument applied to Wigner's original definition: $|\mathcal{P}(x_1, \cdots, x_n; p_1, \cdots, p_n)| \le \left(\frac{1}{\hbar\pi}\right)^n$.

E Wigner

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[9]Remark on units: As defined by Wigner, WFs have units of $1/\hbar^n$ in $2n$-dimensional phase space. Since it is customary for the density operator to have no units, a compensating factor of $\hbar^n$ is required in the Weyl correspondence relating WFs to $\boldsymbol{\rho}$s. Issues about units are most easily dealt with if one works in "action-balanced" x and p variables, whose units are $[x] = [p] = \sqrt{\hbar}$.

Pure-state Wigner functions must obey a *projection* condition. If the normalization is set to the standard value

$$\iint_{-\infty}^{+\infty} dx dp \, F(x,p) = 1 \; ,$$

then the function corresponds to a pure state if and only if

$$F = (2\pi\hbar) \, F \star F \; .$$

These statements correspond to the pure-state density operator conditions: $Tr(\rho) = 1$ and $\rho = \rho \rho$, respectively.

If both of the above are true, then F describes an allowable pure state for a quantized system. Otherwise not. You can easily satisy only one out of these two conditions, but not the other, using an F that is not a pure state.

Without drawing on the Hilbert space formulation, it may at first seem to be rather remarkable that explicit WFs actually satisfy the projection condition (cf. the above Gaussian example, for the only situation where it works, $a = b = 1$, i.e. $\exp\left(-\left(x^2 + p^2\right)/\hbar\right)$). However, if F is known to be a $\star$ eigenfunction with non-vanishing eigenvalue of some phase-space function with a *non*-degenerate spectrum of eigenvalues, then it must be true that $F \propto F \star F$ as a consequence of associativity, since both F and $F \star F$ would yield the same eigenvalue.

Some simple exercises for students to sharpen their QMPS skills. Show the following.

Exercise 1 *Non-commutativity.*

$$e^{ax+bp} \star e^{Ax+Bp} = e^{(a+A)x+(b+B)p} \, e^{(aB-bA)i\hbar/2}$$

$$\neq$$

$$e^{Ax+Bp} \star e^{ax+bp} = e^{(a+A)x+(b+B)p} \, e^{(Ab-Ba)i\hbar/2}$$

Exercise 2 *Associativity.*

$$\left(e^{ax+bp} \star e^{Ax+Bp}\right) \star e^{\alpha x+\beta p}$$

$$= e^{(a+A+\alpha)x+(b+B+\beta)p} \, e^{(aB-bA+a\beta-b\alpha+A\beta-B\alpha)i\hbar/2}$$

$$= e^{ax+bp} \star \left(e^{Ax+Bp} \star e^{\alpha x+\beta p}\right)$$

Exercise 3 *Trace properties.* (a.k.a. "Lone Star Lemma")

$$\int dx dp \, f \star g = \int dx dp \, f g = \int dx dp \, g f = \int dx dp \, g \star f$$

Exercise 4 *Gaussians.* For $a, b \geq 0$,

$$\exp\left(-\frac{a}{\hbar}\left(x^2 + p^2\right)\right) \star \exp\left(-\frac{b}{\hbar}\left(x^2 + p^2\right)\right) = \frac{1}{1+ab} \exp\left(-\frac{a+b}{(1+ab)\hbar}\left(x^2 + p^2\right)\right) \; .$$

Additional exercises may be culled from the first chapter of [20].

There is no need to deal with wave functions or Hilbert space states. The WFs may be constructed directly on the phase space [9, 2]. Energy eigenstates are obtained as (real) solutions of the $\star$-*genvalue* equations [6, 20]:

$$H \star F = E F = F \star H .$$

To illustrate this, consider the simple harmonic oscillator (SHO) with ($m = 1$, $\omega = 1$)

$$H = \frac{1}{2} \left(p^2 + x^2 \right) .$$

The above equations are now second-order *partial* differential equations,

$$H \star F = \frac{1}{2} \left(\left(p - \frac{1}{2} i\hbar\, \partial_x \right)^2 + \left(x + \frac{1}{2} i\hbar\, \partial_p \right)^2 \right) F = EF ,$$

$$F \star H = \frac{1}{2} \left(\left(p + \frac{1}{2} i\hbar\, \partial_x \right)^2 + \left(x - \frac{1}{2} i\hbar\, \partial_p \right)^2 \right) F = EF .$$

But if we subtract (or take the imaginary part),

$$\left(p\partial_x - x\partial_p \right) F = 0 \quad \Rightarrow \quad F(x,p) = F\left(x^2 + p^2 \right) .$$

So $H \star F = EF = F \star H$ reduces to a single *ordinary* differential equation (Laguerre, not Hermite!), namely, the real part of either of the previous second-order equations.

There are integrable solutions if and only if $E = (n + 1/2)\,\hbar$, $n = 0, 1, \cdots$ for which

$$F_n(x,p) = \frac{(-1)^n}{\pi\hbar} L_n \left(\frac{x^2 + p^2}{\hbar/2} \right) e^{-(x^2 + p^2)/\hbar} ,$$

$$L_n(z) = \frac{1}{n!} e^z \frac{d^n}{dz^n} \left(z^n e^{-z} \right) .$$

The normalization is chosen to be the standard one $\iint_{-\infty}^{+\infty} dx dp \, F_n(x,p) = 1$. Except for the $n = 0$ ground state (Gaussian) WF, these F's change sign on the xp-plane. For example: $L_0(z) = 1$, $L_1(z) = 1 - z$, $L_2(z) = 1 - 2z + \frac{1}{2} z^2$, etc.
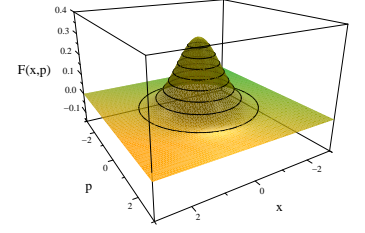
Using the integral form of the $\star$ product, it is now easy to check these pure states are $\star$ orthogonal:

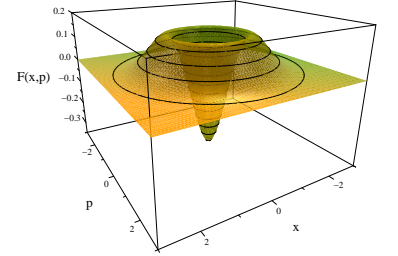$$(2\pi\hbar) \, F_n \star F_k = \delta_{nk} \, F_n .$$

This becomes more transparent by using $\star$ raising/lowering operations to write[10]

$$F_n = \frac{1}{n!} \left(a^* \star \right)^n F_0 \left(\star a \right)^n$$

$$= \frac{1}{\pi\hbar n!} \left(a^* \star \right)^n e^{-(x^2+p^2)/\hbar} \left(\star a \right)^n ,$$
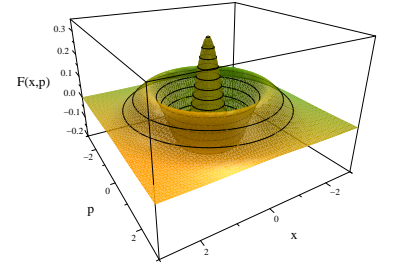
where a is the usual linear combination $a \equiv \frac{1}{\sqrt{2\hbar}}(x + ip)$, and a^* is just its complex conjugate $a^* \equiv \frac{1}{\sqrt{2\hbar}}(x - ip)$, with $a \star a^* - a^* \star a = 1$, and $a \star F_0 = 0 = F_0 \star a^*$ (cf. coherent state density operators).
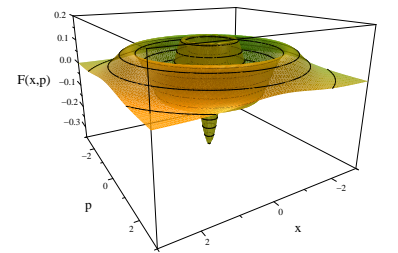

$n = 0$

$n = 1$

$n = 2$

$n = 3$

---

[10]Note that the earlier exercise giving the star composition law of Gaussians immediately yields the projection property of the SHO ground state WF, $F_0 = (2\pi\hbar) F_0 \star F_0$.

   Expectation values of all phase-space functions, say $G(x, p)$, for a system described by $F(x, p)$ (a real WF, normalized to 1) *are just integrals* of *ordinary* products (cf. Lone Star Lemma)

$$\langle G \rangle = \int dx dp \, G(x, p) \; F(x, p) \; .$$

These can be negative, even though G is positive, if the WF flips sign. So how do we directly establish simple correct statements such as $\left\langle (x + p)^2 \right\rangle \geq 0$ without using marginal probabilities or invoking Hilbert space results?

   The roles of positive-definite Hilbert space operators are played on phase space by *real star-squares*:

$$G(x, p) = g^*(x, p) \star g(x, p) \; .$$

These *always* have non-negative expectation values for any g and any WF,

$$\langle g^* \star g \rangle \geq 0 \; ,$$

even if F becomes negative. (Note this is *not* true if the $\star$ is removed! If $g^* \star g$ is supplanted by $|g|^2$, then integrated with a WF, the result could be negative.)

   To show this, first suppose the system is in a pure state. Then use $F = (2\pi\hbar) \, F \star F$ (see Pure States and Star Products), and the associativity and trace properties (see Exercises), to write:[11]

$$\int dx dp \; (g^* \star g) \; F = (2\pi\hbar) \int dx dp \; (g^* \star g) (F \star F)$$

$$= (2\pi\hbar) \int dx dp \; (g^* \star g) \star (F \star F)$$

$$= (2\pi\hbar) \int dx dp \; (g^* \star g \star F) \star F$$

$$= (2\pi\hbar) \int dx dp \; F \star (g^* \star g \star F)$$

$$= (2\pi\hbar) \int dx dp \; (F \star g^*) \star (g \star F)$$

$$= (2\pi\hbar) \int dx dp \; (F \star g^*) (g \star F)$$

$$= (2\pi\hbar) \int dx dp \; |g \star F|^2$$

$$\geq 0 \; .$$

In the next to last step we also used the elementary property $(g \star F)^* = F \star g^*$.

   More generally, if the system is in a mixed state, as defined by a normalized probabilistic sum of pure states, $F = \sum_j \mathcal{P}_j F_j$, with probabilities $\mathcal{P}_j \geq 0$ satisfying $\sum_j \mathcal{P}_j = 1$, then the same inequality holds.

---

[11]By essentially the same argument, if F_1 and F_2 are two distinct pure state WFs, the phase-space overlap integral between the two is also manifestly non-negative and thus admits interpretation as the transition probability between the respective states:

$$\int dx dp \, F_1 F_2 = (2\pi\hbar)^2 \int dx dp \, |F_1 \star F_2|^2 \geq 0 \; .$$

Correlations of observables follow conventionally from specific choices of $g(x, p)$. For example, to produce Heisenberg's uncertainty relation, take

$$g\left(x, p\right) = a + bx + cp \ ,$$

for arbitrary complex coefficients a, b, c. The resulting positive semi-definite quadratic form is then

$$\langle g^* \star g \rangle = \begin{pmatrix} a^* & b^* & c^* \end{pmatrix} \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle \\ \langle x \rangle & \langle x \star x \rangle & \langle x \star p \rangle \\ \langle p \rangle & \langle p \star x \rangle & \langle p \star p \rangle \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \geq 0 \ ,$$

for any a, b, c. All eigenvalues of the above 3×3 hermitian matrix are therefore non-negative, and thus so is its determinant,

$$\det \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle \\ \langle x \rangle & \langle x \star x \rangle & \langle x \star p \rangle \\ \langle p \rangle & \langle p \star x \rangle & \langle p \star p \rangle \end{pmatrix} \geq 0 \ .$$

But

$$x \star x = x^2 \ , \qquad p \star p = p^2 \ , \qquad x \star p = xp + i\hbar/2 \ , \qquad p \star x = xp - i\hbar/2 \ ,$$

and with the usual definitions of the variances

$$(\Delta x)^2 \equiv \langle (x - \langle x \rangle)^2 \rangle \ , \qquad (\Delta p)^2 \equiv \langle (p - \langle p \rangle)^2 \rangle \ ,$$

the positivity condition on the above determinant amounts to

$$(\Delta x)^2 (\Delta p)^2 \geq \frac{1}{4}\hbar^2 + (\langle xp \rangle - \langle x \rangle \langle p \rangle)^2 \ .$$

Hence Heisenberg's relation

$$(\Delta x)\left(\Delta p\right) \geq \hbar/2 \ .$$

The inequality is saturated for a vanishing original integrand $g \star F = 0$, for suitable a, b, c, when the $\langle xp \rangle - \langle x \rangle \langle p \rangle$ term vanishes (i.e. x and p statistically independent, as happens for a Gaussian pure state, $F = \frac{1}{\pi\hbar} \exp\left(-\left(x^2 + p^2\right)/\hbar\right)$).

W Heisenberg

A Classical Limit

The simplest illustration of the classical limit, *by far*, is provided by the SHO ground state WF. In the limit $\hbar \to 0$ a completely localized phase-space distribution is obtained, namely, a Dirac delta at the origin of the phase space:

$$\lim_{\hbar \to 0} \frac{1}{\pi\hbar} \exp\left(-\left(x^2 + p^2\right)/\hbar\right) = \delta\left(x\right) \delta\left(p\right) \ .$$

Moreover, if the ground state Gaussian is uniformly displaced from the origin by an amount (x_0, p_0) and then allowed to evolve in time, its peak follows a classical trajectory (see Movies ... this simple behavior does *not* hold for less trivial potentials). The classical limit of this evolving WF is therefore just a Dirac delta whose spike follows the trajectory of a classical point particle moving in the harmonic potential:

$$\lim_{\hbar \to 0} \frac{1}{\pi\hbar} \exp\left(-\left((x - x_0 \cos t - p_0 \sin t)^2 + (p - p_0 \cos t + x_0 \sin t)^2\right)/\hbar\right)$$

$$= \delta\left(x - x_0 \cos t - p_0 \sin t\right) \delta\left(p - p_0 \cos t + x_0 \sin t\right) \ .$$

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